

# **Multiscale Issues and Simulation-Based Science and Engineering for “Material-by-Design”**

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**Abstract:**

Through actively participation, engagement and steering community activities and literature survey, this project is to evaluate the progress and the state-of-the-art of multiscale research issues, and to arrive at a strategy for planning and execution of programs to achieve the vision of “material-by-design”. A key part of this effort has been to examine modeling at the mesoscale. A report on a recent modeling workshop that we co-organized is included as an appendix.

**Introduction:**

Coupled the scientific advancement with and the computing power increase during the past several decades has made unprecedented opportunity for scientists to pursue better understanding of the physics fundamentals across different length and time scale in the multidisciplinary context. With this understanding, it enables the engineers to design more efficient systems using the new computing tools that are being developed. At the same time, the advancement in nanotechnology, biotechnology and information technology have given the scientists and engineers a new challenge of uncovering the connectivity in physics and chemistry from one scale to another, from atomic to astrophysics, and to design systems from the “bottom-up” using the knowledge and understanding of the multiscale fundamentals. It is under this spirit that the academic community as well as the funding agencies has been energized. The latest effort is a joint commissioned study by the US National Science Foundation, Department of Energy, National Institute of Health, NASA and the Department of Defense to World technology Evaluation Center, Inc. to look into this issue nationally and globally. After near two-years of deliberation, a report entitled “International Assessment of Research and Development in Simulation-Based Engineering and Science” has been completed (Reference).

During the same time, many academicians and government funding agencies have already taken their own initiatives of looking at the multiscale issue from his/her discipline or knowledge base. Much progress has been made in this fashion. However, these efforts further point out the need of a common-based understanding of the multiscale understanding at a cross-discipline level.

The goal of this study is to investigate the technology development of the multiscale research from a narrower view point, i.e. from micro- to meso- to macroscale. It is intended to further the notion of “materials-by-design” through better understanding of the multiscale fundamentals in their scale effects and the handshake relationship when one marches from one scale to another. It is a paper study and the product will be a state-of-the-art evaluation and the proposed strategy for program planning and execution.

## **Approaches:**

There will be two major tasks of the proposed research. The first task is to conduct a state-of-the-art assessment of the multiscale efforts from micro- to meso- to macroscale with a focus on the “materials-by-design”. The second task is to generate a strategy for the researchers and for the funding agencies’ reference.

Literature search and direct communication with those in the research community and funding agencies is the way to gain insight into this area. For example, the commissioned World Technology Evaluation Center, Inc (WETC) report will be carefully evaluated to extract areas of relevance that are within this study scope. Specifically, other areas of atomic scale or astrophysics scale areas are not within the micro-to macro-scale for the purpose of “materials-by-design”. Direct communication includes face-to-face meeting or other forms of communication with those who have been working on this issue. For example, Prof. Tinsley Oden of the University Texas at Austin has been an active researcher in this area himself and has also served as the chairman of the fact finding committee of the subjected study. Therefore, Prof. Oden has not only the knowledge of the on-going effort in this area but also has been visiting many of these researchers in and outside the United States.

Participating or organize workshop that focus on the scale of the present interest is the second activity to achieve the program goal. Attending specialty workshops and participating deliberation to stimulate insightful discussion on multiscale issues is needed. Additionally, coordinating with the funding agencies and the research community, it is proposed to proactively organizing focused workshops for working on the scientific issues related to the subjected matters, and toward a workshop output/strategy for funding agency’s planning and execution. The unique advantage of the focused workshop is to provide an opportunity where the selected leading researchers to have in-depth discussions on the scientific opportunities, issues, limitations and to arrive at the observations and the way-forward in a truly cross-discipline manner. The multidisciplinary nature of the multiscale problem is a cross-discipline issue and it can only be addressed properly in the multidiscipline fashion; i.e., physics, chemistry, mathematics, engineering, materials and systems.

## **Accomplishments:**

## **Task one**

Multiscale research is not new; people from different community have been engaging multiscale research for the purpose of fundamental technology advancement/understanding and of new materials design. However, the approach has always been the one that starting from a specific discipline, i.e. within specific length and time scale, and trying to connect to the neighboring scales within that specific discipline frame work. In terms of the treatments, moving from micro to macro usually goes from the discrete to continuum, i.e. molecular dynamics or similar treatment to continuum mechanics. Typically, material science plays the middle role but treatments are mostly limited to geometric centric/emphasized, i.e. grain, phase and interface. On the other hand, mechanics treatment has been centered on homogeneous and continuity relationship. In doing so, most of the time, one is forced to give-up the chemistry and physics fundamentals at the interfaces and its effects among different phases (interphases) that make up the material system. The treatment of the cross scale challenge has been done from its own discipline point of view. For example, the mechanics treatment of the material science issues has been based on the continuity relationship with a very limited modification to include variables such as dislocations, grain size and grain structures. Little to no consideration has been given to the physics or chemistry effects such as electron density, quantum effects that do influence the materials behavior greatly especially when physical size becomes very small, i.e. to the nano-level.

Historically, this relatively simplified approach has been used is because there is very little cross disciplinary interaction culture, and there are limited computing power to consider all aspects of the problem. For certain classes of problem, the historical treatments have been proven sufficient. However, in order to achieve the so-called "materials-by-design" vision, the legacy approach will not take us there. Most importantly, we are in the middle of integrating nanomaterials into the micro and macro material systems to take advantage of what the nanotechnology has to offer. For these cases, it is not unreasonable to speculate that the quantum effect at the interfaces and its effects among the different phases play an very important role in the behavior, properties and fabrication of these materials systems; therefore it would be wrong not to consider the quantum effects.

Additionally, the material is a system that is neither homogeneous nor behaves deterministically. The historical deterministic treatment was used because of the limited knowledge and tools during the early days of mechanics and materials theory development. With the theory and the computing capability we have today we are in a position to treat the true statistical nature of the

material behavior. Only by doing this way, one then can realize the “material-by-design” potential. Specifically, any realistic treatment must consider the stochastic nature of the material complexity.

The example given above is between the material science and mechanics. However, to understand the materials and there intended applications, one sometimes must go one level down in scale to reach molecular dynamics level. In this case, one is facing with the reality of having chemical engineering, material science and mechanics discipline to work as a team. The reality is that all three disciplines have their own culture, terminology and emphasis. The only way to move across discipline boundary is to have the team work together, and have the team effort moves from one-scale-to-the-next to assure that important physics or chemistry fundamentals are not lost from any simplification process. Specifically, when moving from the finer scale to the next, one must be assure to establish proper handshake relationships which are correct in the fundamental physics and chemistry sense. In order for us to realize the "materials-by-design" potential, one must treat it as a multi-scale problem and must be work collectively on a cross-discipline manner by the experts from all these disciplines, physics, chemistry, computing science and modeling, material sciences and mechanics.

Another aspect of this process is the experiments and computing. In this case, the experiments is more than verification, it is the needed tool for assisting theory development. With the proper understanding of the handshake relationship on a multiscale problem, one can march from one scale to another with the assurance that the fidelity and truthfulness of the physics and chemistry are handed over to the next scale for the problem and applications intended. The mechanism of doing this task depends on the success of the model development and experimental characterization. In this case, dealing with the proper experiment method development and computation related efforts are not trivial matters. The proper algorism must be developed to assure a faithful representation of the multiscale problem in hand that not only contains property fundamentals of chemistry, physics, material sciences and mechanics, but numerically stable and effective. A careful balance must be maintained between the material/mechanics effort and the numerical concentric computing effort. Both are essential and require extensive research effort but neither can be successful without the other. In fact, this wrong assumption has been one of the major problems in multiscale research, i.e., simulation sometimes is viewed and referred as only computing simulation without physics or other way around. Having these disciplines working as an integrated team is the only way to assure success.

The limitation of the computing power is still a major issue because the needed granular level and fidelity of computation. Because of the smaller scales oftentimes have the most impact on a material properties, fabrication and performance; one is tempted to model the material systems at the lowest granularity. Unfortunately, even with today's computing power, we are in no position to do so. The computing science specialist's contribution is to reduce the degree of freedom of the problem and to make it solvable, and faithful represent the problem at hand.

Computing infrastructures development is another important element in the "simulation based engineering and science" context. It is more than the hardware development. Since this is beyond the scope of this research, it is only mention at here but no details are spelled out.

Since one of our goals is to learn from the goodness of the biological systems, one must also have life sciences experts on the team to help us to understand the structure, function and processing (not structure alone as we have done mostly in the biomimetic research) of the nature materials for us to mimic these material systems effectively.

In addition to going through the literature search and carrying on extensive personal interactions with those experts who are experts in their own field, an invitational workshop was organized and held. Instead of addressing all the length and time scales ranging from atomic physics to astrophysics, the workshop was focused on the micro- to meso- to macro-scales. This workshop "Challenges in Mesoscale Mechanics of Complex Materials" was held at Vancouver, Canada. It was a small invitation only gathering, around 40 people from the academia in the US and other countries in the Asia region. All attendees were invited because of their technical credential. The funding agencies representatives were the National Science Foundation, National Institute of Science and Standards, Air Force Office of Scientific Research, AOARD, the US Army, and the Academy Sinica of Taiwan (see Appendix).

The discussion and observation from the workshop on the state-of-the-art and the way ahead are contained in the workshop write-up. Specifically, the traditional effort from micro- to meso- to macro-effort has been focused on the "geometric morphology" in a more or less deterministic way. Little attention has been given to the fundamental aspects of the physics and chemistry relationship when marching from one scale to another. The treatment of multiscale has been limited within each of the discipline field, i.e. molecular dynamics to material sciences to solid mechanics as the case may be. Therefore, the take away message from this workshop is that one should treat the "geometry morphology" and also to include the fundamental physical and chemistry morphology at the interfaces and its effects on the inter-phase relationship among

different scale and different phases of the substructures. In this case, the problem has become a multi-discipline problem where only a close collaboration among the physics, chemistry, material sciences and mechanics researchers can realize the true solution of the multiscale problem. Most importantly, it is no longer a deterministic problem; a stochastic approach must be invoked to faithfully address the non-deterministic aspect of the problem.

## **Task 2:**

Because of the unique aspect of the multiscale effort, i.e. people from various disciplines having different history, culture, terminology, confront zone and emphasis, a means of a true cross-discipline effort is a must to assure success. The cross-discipline team is different from the conventional multidiscipline team where different experts work on coordination but with only limited collaboration. The perquisite of this cross-discipline team is that each team member must have some technical depth in the other related disciplines that enables him not only to appreciate the contributions made by the others but also to work the problem with others in a truly integrated fashion. For examples, the mechanics and materials specialists must understand and work with the computing simulation specialists to understand the computing related issues and approaches. It would be a mistake to assume that one can develop the most efficient, robust and faithfully representative models without knowing computing science insight. On the other hand, it would be a total disaster for the computing specialists to model the equations without correct inputs from the mechanics and materials specialists.

Building this cross-discipline team is the most challenge tasks because it requires the experts not only from the different discipline but also from different organizations to work integrally toward a common objective. Therefore, technical collaboration as well as institutional collaboration is equally important elements for success. Additionally, even with the better understanding on the related physics, chemistry, materials, mechanics and advancement in computing simulation we have today, the problem is still too vast to arrive at any generic solution. Therefore, one must focus down onto the problems that are manageable. For example, composite, metals or electronics all have different characteristics and utilities, the fundamental physics and chemistry as well as the simulation model development effort differs. The handshake relationship among scales must be sound to satisfy the physics and chemistry fundamentals. Since the ultimate goal is “material-by-design”, the parameter space must be clearly defined through intense interaction among the team members through rigorous simulation models and experimental verifications. It is through this iterative approach; one can not only build manageable simulation



models for prediction but also discover/arrive at proper physics and chemistry representations for the material systems of interest.

As for the funding agency, a working group for coordination is a must because it is a huge endeavor and leveraging each other's effort and resources is a must. Most importantly, the fundamentals developed from different agency funded effort can easily be modified/adopted by the others for solving agency unique problems.

Because of the important of the "Simulation based Engineering and Science", nearly all funding agencies are either on preparation or getting started to build program plans for implementation. At the top level, there are several studies sponsored by the Office of the Science and Technology Policy (OSTP) on this topic. The one related to the subjected issue is on-going and is called "Simulation-Based Engineering and Sciences for Discovery and Innovation." This is a fast track study and the concentration is on materials and weather. The draft report from this OSTP study on materials is aligned with the Vancouver workshop but with an emphasis on solid materials. At the working level, there is an on-going Army Research Laboratory sponsored National Research Council study conducted through the National Materials Advisory Board on materials of Army's interest - "Opportunity in Protection Materials Sciences and Technology for Future Army Applications". These two are examples on materials. Other studies on multiscale simulation are ranged from fundamental physics simulation to astrophysics.

With the definition of the state-of-the-art and the challenges and issues, the other effort needed is programmatic, i.e., advocating and planning the coordinate effort among all the constituents - funding agencies in the US and abroad. A presentation was given to the Defense Basic Research Coordination Group (DBRCG) and received group endorsement to work and coordinate this effort with other government organizations. DBRCG membership is made of the Director the Air Force Office of Scientific Research, Director of The Army Research Office, The Chief Scientist of the Office Of naval Research, plus appropriate representatives from the Defense Threat Reduction Agency and Defense Advanced Research Project Agency. An informal coordination group made of National Science Foundation, National Institute of Science and Standard and DoD has been formulate for program advocacy, coordination and leveraging. The foreign countries participation will be through the DoD and NSF foreign offices, such as AFOSR's AOARD, EOARD, Office of Naval Research Global and the Army Research Laboratory and other Army foreign establishments. The next step is for this group to meet up

with the OSTP to advocate not only the topic issues but also stress the fact that we are working together on this important national initiative.

### **Payoff:**

The present Air Force inventory must possess two major attributes (1) readiness to meet the needs and (2) high performance standard to defeat the adversary. In this case, maintaining the state-of-health of the system and the sustaining the systems effectiveness requirement are the keys to assure durability. More importantly, the designed superiority in our systems must not be comprised by the lack of functionality due to system degradation. On the other hand, for the future Air Force systems, the scientific and technology communities do play a major role in designing robustness and superiority into them through technologies and innovations. Regardless old or new, for these systems in our inventory and those still on the drawing board, the simulation based design and maintenance are the only effective means to achieve robustness and high performance. Since the multiscale knowledge is a must for developing the simulation models from one-scale to another, from atomic scale to overall system scale, the fundamental understanding of multiscale issues and the methodology of physically based hand shake relationship from one scale to another becomes the make-and-break factor to maintain and/or enhance Air Force systems performance. With it, one can have readiness, robustness and superiority. Without it, one is left with the outdated incremental technology and tools without possibility of achieving innovation for achieving major advancement in readiness or performance.

### **Summary:**

Multiscale fundamentals and its applications to the simulation based engineering design and performance improvement are the opportunity as well challenges presented to the engineering and science community for achieving “material-by-design”. This report gives an evaluation of the state-of-the-art of the multiscale research and the way ahead to realize the “material-by-design” potential. Additionally, it also laid out the landscape among government funding agencies activities for address this important challenge.

### **Reference:**

“International Assessment of Research and Development in Simulation-based Engineering and Science”, World Technology Evaluation Center, 2009.

## **Appendix:**

Report from Vancouver Invitation Workshop on Mesoscale Mechanics of Complex Materials (September 2009).

### **Challenges in Mesoscale Mechanics of Complex Materials**

Reported by

Wing Kam Liu, Northwestern University, and Zhiquag Suo, Harvard University

Materials often exhibit a high degree of complexity because of the interaction of processes at the extreme and intermediate scales. For conciseness we will call these complex materials. While continuum mechanics governs the behavior of a material at macroscopic scales, and quantum mechanics governs the behavior of electrons at the Angstrom scale, the behavior of a material often crucially depends on the bridging of these scales through the intermediate scale, the *mesoscale*. Key physical/chemical/biological phenomena take place in the mesoscale, and they cannot be properly described by continuum mechanics or quantum mechanics alone. The interactions between morphologies (material structures) and time scales associated with the mesoscale in a multi-physics environment often create new phenomena and material properties dependent on both fine and coarse scale behavior. Thus the mesoscale is critical in the translational research of complex materials.

The mesoscale behavior of a material is governed by both continuum behavior and pronounced surface effects where *interphase properties* must be accounted for and *interfacial interaction* must be understood. In fact, when decomposing a system into its constituent scales, *the mesoscale acts as the link between the continuous and discrete portions of the scale spectrum*. Sitting at the threshold between continuous and discrete time and space scales, the mesoscale is home to a diverse set of governing physics.

*The mesoscale acts as the link between the continuous and discrete portions of the scale spectrum. Thus mesoscale mechanics plays a critical bridging role in the multi-resolution paradigm. An understanding of the mesoscale is essential in predicting the behavior and enabling design of complex materials.*

Due to the multitude of physics, complex meso-structures, and mankind's frequent inability to match experiments and simulations, mesoscale mechanics of complex materials exhibits a great deal of complexity and stochasticity which are still beyond the current state-of-the-art knowledge base. The field offers challenges that require significant advancement and the development of new theoretical background.

*We need a unified science-based, mathematical, and computational framework for mesoscale mechanics that melds new basic theories, numerical algorithms, and computing architectures with fundamental science.*

“Mesomechanics” may be one of the most important links in the scheme of multiscale efforts for engineered systems and beyond. In reality, we are not able to build a unified physics-based theory to march from the atomic scale to the astrophysics scale, or even the macroscopic scale of consumer products, aircraft, or biological cells, due to the complex interplay between mechanisms at each scale, the disconnect between academics from the physical sciences, the life sciences, and engineering, the difficulty in theory development to bridge so many scales, and perhaps most importantly the insurmountable computational resource requirements. Nevertheless, because of the advancement in fundamental understanding and in computing capability, we are in a good position to attack a subset of the multiscale problem, i.e. to connect material sciences to mechanics to systems and structures. For example, nanotechnology has become an enabler for designing smart systems/structures that mimic life science entities. In nano-reinforced systems, the interfaces between material phases exist from nano- to macro-domains, where a firm grasp of characteristic length and time quantities are of the essence. Nano-systems are no longer a ‘mechanics only’ interface problem; fundamental quantum behavior may have to be investigated for us to realize the nanotechnology potential, first through understanding *interface* and *interphase* material behavior at the atomistic level and secondly through wielding this knowledge to unlock multiscale prediction. If multi-resolution analysis mutates to predictive science, ensuing radical performance improvements in macroscopic structures and functional systems will occur.

As was demonstrated in the workshop on Mesoscale Mechanics of Complex Materials, work in mesoscale mechanics connects fine resolution material morphology to functionality across time and space scales. That is, the structure of a complex material's mesoscale dictates its bulk properties, which in turn control system performance. Candidate materials in which the study and theoretical development in mesoscale mechanics can yield great benefits include metals and alloys, micro- and nano-composites, soft materials like polymers, piezo- and thermo-electrics,

biological tissue, and beyond. Through an understanding of these complex materials, significant societal impact can be realized in applications in Energy (high efficiency, low cost bio-inspired solar cells, solid state fuel cells, batteries, energy harvesting, meso-photosynthesis, . . . .), Biology (disease diagnostics, drug delivery, implants, muscle imitation, prosthetics, . . . .), and Materials (fatigue life prediction, damage prediction, smart materials, self-healing alloys, reusable adhesives, bio-inspired materials, . . . .).

Many of the above components exist but are operating independently. To name several examples, research is being conducted on (a) modeling and simulation of hard/soft asperity on surface interaction to mimic nanoindentation or nanoscratching, (b) theory of dislocation density in metal microstructures to describe the time evolution of damage in inhomogeneous mesoscale materials, (c) simulation and theory of atomistic objective structures via density functional theory to extrapolate behavior at the larger mesoscopic scale, (d) micromechanical constitutive models coupling theory and experiments of large deformation of viscoelastic soft materials, (e) multi-physics theory and computation of soft material micro-actuators where mechanical deformation is induced by temperature, voltage, pH, or magnetic potential, (f) coarse graining numerical methods for efficient treatment of interfacial effects in polymer nanocomposites via molecular dynamics, (g) theory of processing mechanics of multifunctional composite nanofibers via electrospinning to garner better mechanical mesoscale properties, (h) numerical modeling to validate and enhance theory of deformable particles in laminar flow with applications to amorphous waste transport or blood flow in animals, (i) multi-resolution continuum mechanics and its cyber-enabled computational framework for complex materials, and (j) microscale polymer gel-silicon interaction to pioneer stretchable electronics that will allow conforming equipment in many applications from military to medical, and the list goes on.

The aforementioned applications require rigorous explanation advances in theories and methods applicable to a wide range of linked time and length scales via new mesoscale mechanical theory. New theories are paramount to the science and engineering community's understanding of mesoscale phenomena. As can be seen from the examples above, the mesoscale is the link between the discrete length scales of atomistic behavior and continuous length scales, where discrete behavior is averaged to produce desired macroscale behavior, or in traversing the opposite direction, physical behavior of a system at the continuous macroscales can only be fully understood by delving into the discrete length domain. That is, in a multi-resolution system, nested fine resolutions inform macro-domain theory. *The mesoscale serves as the cornerstone*

*for codependence of discrete behavior with continuum behavior* since it is the scale at which these two portions of the length spectrum are in direct, *observable* contact.

## **Mesoscale Concepts**

Delving further into re-examination of the mesoscale yields two distinct concepts by which to explain the phenomena taking place at this length and time scale. These will be explained one by one.

Due to the coexistence of atomistic and continuum theories meeting in the mesoscale, the random fluctuations of fine scale material structures create notable stochastic mesoscale anomalies realized as meso-voids, imperfect grain surfaces, or contact interfaces with imperfect bonds. These stochastic anomalies are introduced during material manufacturing and create a random meso-structure morphology which gives rise to ***geometry-morphology based mesoscale mechanics***. In this concept, the complexity of the mesoscale arises from the complexity of the morphology. Put simpler, if all phases in a material system were ideally processed, ideally bonded, and ideally smooth at their domain boundaries, the mesoscale would be more easily explained with the current modeling techniques available to the analyst. No such utopia exists, however, so the complexity of the mesoscale is attributed to the random nature of mesoscale geometry in this mode of thought. In this concept, the analyst's inability to properly model, by mathematics, computations, and experiments the degree of stochastic imperfection in material constituents is the source of mesoscale complexity.

Besides stochastic meso-structure geometry, the coexistence of discrete mechanics and continuum mechanics in the mesoscale gives rise to marked interface and interphase effects whose physics cannot be fully described by the analysis methods, both theoretical and computational, of one particular domain. The competing physics in the mesoscale, therefore, give rise to ***science-based mesoscale mechanics***. For example, a continuum description of a mesoscale unit cell will never capture the alteration of mechanical properties in a region of the matrix phase surrounding an inclusion. Conversely, mesoscale unit cells must consist of far too many atoms (so as to be statistically homogeneous) to allow explicit simulation of the mesoscale via quantum mechanical or molecular dynamical methods. In fact, the mesoscale behavior occurs at length *and* time scales inaccessible by discrete descriptions alone so even static properties may be difficult to obtain. As opposed to geometry-morphology based mesoscale mechanics, where the analyst assumes he has sufficient knowledge and understanding of key system physics to explain the mesoscale behavior *if* he knew the morphology (while noting this is an impossible

task), a follower of science-based mesoscale mechanics claims that underlying physical mechanisms describing the system must be re-evaluated.

### **Added Complexity – Experiments and Uncertainty**

Multi-resolution experiments play a crucial role in both concepts. For instance, within geometry-morphology mesoscale mechanics, the inability of the experimentalist to accurately image the meso-structure in a 3-dimensional environment at fine enough spatial and temporal resolution creates a large amount of uncertainty in the analysis. Oftentimes, both the structure (spatial portion) and the evolution (temporal portion) of the mesoscale are not well characterized in an experiment. From a science-based mesoscale mechanics perspective, limited mesoscale experiments provide valuable benchmarked data for which to reveal areas of model insufficiencies due to misunderstood physics.

Regardless of the philosophical approach to tackling mesoscale mechanics applications, a high degree of complexity can never be avoided. This complexity may be handled through ever-increasing computational power and better numerical algorithms, more focused and sensitive experiments, and perhaps most importantly, a unified theoretical approach to explaining mesoscale behavior. Undoubtedly, the challenges that can greatly reduce the complexity inherent in describing the mesoscale require a huge amount of brainpower, man hours, and money. Since engineers and scientists operate with finite time and budgets, they must recognize that understanding all the details of mesoscale mechanics is impossible. *Choosing and subsequently understanding important mesoscale details is at the heart of successful multi-resolution analysis.*

In working to achieve this feat uncertainty is widely introduced into the system and propagated among the nested scales. *The analyst, therefore, must not ignore the effects of uncertainty in the mesoscale where multiscale complexity reaches its zenith.* The stochastic nature of material properties exists in every scale of physical events and becomes increasingly important in and around the mesoscale. Uncertainty in any complex multiscale system arises from 3 sources: (1) the random fluctuation of microstructure morphology statistics based on uncertainty in material manufacturing, (2) lack of knowledge from insufficient small scale experimental procedures and misunderstood physics, and (3) the lack of computational resource that prevents the analyst from simulating large enough micro-domains. These three sources fit into the two mesoscale analysis concepts given prior to this paragraph. Uncertainties propagate from one scale to the next and from one physical event to another and all affect the response of interest in different ways. The multiscale multi-physics nature in the mesoscale materials calls for the need to develop new

mathematical theories for uncertainty representation, quantification, and propagation. With uncertainty properly quantified in a multiscale system, the analyst can *predict the macroscopic system behavior with confidence*, which is the underlying goal of multiscale analysis.

### **New educational approach in computational science and engineering**

The new commercial and open source packages for simulation and analysis, as well as the legacy codes handed down from student to student within research groups, attack complex problems in mesoscale mechanics with sophisticated computational algorithms. This permits students to become quickly involved in cutting-edge research with computational tools. Concurrent with this increase of computing power was the development at several top schools of many new courses in computational methods, computer science and numerical algorithms. While the goal of these courses was to improve our students' abilities to use numerical simulation and analysis in their research, the reality is that there is a growing chasm between graduate researchers who know what transpires in these large software packages and those who use these computer codes as black boxes. A disadvantage of turn-key packages and legacy codes is that students often do not understand the limitations of the codes. Moreover, students are often unable to improve their codes by adding to or correcting the underlying physics, cannot improve the numerical algorithms, and cannot fully interpret the large output files produced. These three shortcomings can be overcome by teaching mesoscale theory alongside computational mechanics and numerical methods.

The mesoscale offers a unique forum for new educational approaches in science and engineering. Specifically, the variety of physics present allows students interested in diverse topics such as energy, biology, materials, physics, and mathematics to come together in an interdisciplinary sense and tackle a common problem. The advancement of predictive science is potentially critical to the simulation and design of new and complex “engineered” systems in a variety of applications across an array of domains like microsystems, biological systems, energy generation and consumption systems, nuclear systems, climate modeling and control, and efficient manufacturing. As such complex systems require the integration of a diverse set of disciplines that come together at the mesoscale, and the sophisticated multi-physics simulations, there is a need for discovering, developing, and teaching the common principles and techniques underlying this new paradigm. Specifically, future success requires unified software and algorithmic frameworks for integrating models and code from multiple disciplines, systematic and comprehensive treatment of the uncertainties inherent in such models, and risk-based decision



making to enable highly confident predictions and reliable design. Since highly interesting phenomena occur in the mesoscale, developing these new teaching methods in conjunction with mesoscale mechanics theory ideally suits researchers and students alike.

## **Conclusions and recommendations**

A central and unifying aim of the mechanics of materials is to relate macroscopic behavior of materials to microscopic processes. The recent focus on the mesoscale mechanics of complex materials results from two great advances. First, nanotechnology has enabled structures to be fabricated efficiently with well-defined nanoscale features. Second, computational technology has created an unprecedented opportunity to simulate complex behavior.

Using these advances in fabrication/manufacturing and computational resource, researchers may begin to confront the translational challenges associated with *science-based mesoscale mechanics* while not overlooking *geometry-morphology based* complexity. To begin this feat, the ambitious researcher must first partition the inner workings of the mesoscale into two categories: the (relatively well) known, and the unknown. In the known region the researcher is confident with his theoretical model and computational capability, yet it is in the unknown region where secrets lie for the taking and scientific discovery awaits. For example, in the unknown region, pronounced interfacial effects may be misguided by empirical interatomic potentials, interphase material properties may be responsible for new viscoelastic responses, or nano/micro particle surface profiles may govern the reinforcement strength and toughness. These hypotheses are tested by a focused brainstorm of what microstructure characteristics, fine-coarse interaction, and physical mechanisms are unexplored and thus remain unknown.

The broad field of mesoscale mechanics involves a wide variety of complex materials, including traditional hard materials like metallic alloys and ceramics; soft materials like polymers, composites, and biological tissues; and emerging materials like active materials, adaptive materials, biomimetic, and bioinspired materials. *All these materials contain unknown meso-regions awaiting explanation and understanding.* The workshop specifically identified three emerging sectors where mesomechanics are expected to be of vital importance: the biomedical industry, alternative energy industry, and multifunctional materials. For the nascent alternative energy industry, mesomechanics can contribute to the development of novel devices for energy harvesting, and materials for the next generation energy industry that aims to lower global consumption. For the biomedical industry, mesomechanics is currently being applied for the development of non-invasive disease diagnostics, surgical planning, drug delivery, implants, and

tissue engineering. For the multifunctional materials industry, mesomechanics principles are helping to develop noise reduction technology via actuation, bio-inspired smart material systems having self contained diagnostic, prognostic and self-healing capability, neuroscience and computing based human performance measurement and training capability, novel microsystems, and phononic crystals for simultaneous vibration isolation and energy harvesting, etc.

Many complex materials require multi-scale and/or multi-physics research, collectively called a multi-resolution framework, to connect structure to properties and ultimately to function. The workshop encourages continuing focus on the development of multi-resolution methods, particularly for hard and soft materials and for composites containing both hard and soft phases. For polymeric materials, there remain significant challenges to molecular dynamics modeling of time-dependent processes such as viscoelasticity, poroelasticity and nonlinear viscoelasticity. Mechanism- and science-based continuum theories of polymer that refer back to the polymer structure are needed for tailored design.

In summary, mesoscale mechanics is rich in untapped knowledge. The unique amalgamation of the discrete length spectrum and its quantum principles with the continuous length spectrum and its continuum principles creates an area whose evolution can only be understood through the marriage of advanced *theoretical development, exploitation of computational methods, and non-traditional experimental validation*. That is, independent from one another, theory, computation, or experiments will not unveil mesoscale science and engineering. Theory must account for limited computational power while computations must affirm the undoubtedly risky theories expected to advance from mesomechanics studies. To forge ahead in research in mesomechanics, one must treat theory, computation, and experimental validation as inseparable foundations upon which future knowledge is built.